COMMENTS

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Comment on ''Electrical transport in junctions between unconventional superconductors: Application of the Green's-function formalism''

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Effects of surface pair breaking, entirely neglected by M. P. Samanta and S. Datta [Phys. Rev. B **57**, 10 972 (1998)], is quite important in considering surface (or interface) quasiparticle bound states and associated characteristics of junctions involving unconventional superconductors. The whole class of bound states with nonzero energy is simply omitted within the framework of the approach, using uniform spatial profile of the order parameter up to the interface. The contribution of these bound states (as well as midgap states) to current-voltage characteristics of the SIS tunnel junctions were studied in our earlier article. Dependence of midgap state contribution to the Josephson critical current upon crystal to interface orientations is shown as well to be fairly sensitive to the effect of surface pair breaking.

In a recent article,[1] Samanta and Datta considered theoretically electrical transport of junctions involving unconventional superconductors. In particular, they discussed contributions to junction properties from midgap surface states, that arise in *d*-wave superconductors due to sign change of the order parameter. They pointed out that the effect of midgap states is most prominent for weakly coupled junctions (tunneling limit), concentrating in this respect mainly on the first-order theory in transmission coefficient. In evaluating electric current across the junction the authors[1] neglected from the very beginning all the effects of surface pair breaking, considering order parameters on both sides of the junction to be equal to their bulk values up to the junction barrier plane. In this Comment we demonstrate that the approximations[1] lead to incorrect results for unconventional superconductors, since effects of surface pair breaking is of crucial importance for the *I*-*V* characteristics of tunnel junctions, especially due to the existence of surface quasiparticle states with nonzero energy. Also we point out that correct theory of current-voltage characteristics of tunnel junctions involving anisotropically paired superconductors was developed earlier in Ref. 2.

In contrast to *s*-wave isotropic superconductors, *d*-wave superconductors are known to be quite sensitive to any inhomogeneities (impurities, surfaces, interfaces). In particular, the order parameter turns out to be substantially suppressed on the tunnel barrier plane for many of crystal to surface orientations. Several important experimental methods used for studying the anisotropic structure of the order parameter, for example, tunneling measurements are, in turn, fairly sensitive to the superconducting properties close to the surface of the sample. The effects of anisotropic pairing on the tunneling density of states (the local quasiparticle spectrum at the surface), the Josephson and quasiparticle current of SIS and SIN tunnel junctions were theoretically studied by taking account of surface pair breaking and quasiparticle surface bound states in Refs. 2–8.

Our main assertion is that the whole class of surface quasiparticle states is omitted in Ref. 1 due to the disregard the surface pair breaking there. Spatial profile of the order parameter suppressed near the surface, can be considered as an effective potential well for quasiparticles. Andreev reflection processes along with the conventional reflection from the surface, can result in forming quasiparticle bound states (Andreev bound states) localized near the surface within the characteristic length roughly of order of the superconducting coherence length. Quasiparticle surface bound states with nonzero energy are present for an impenetrable wall in the case of surface pair breaking and not for a uniform spatial profile of the order parameter. Only midgap surface states, having supersymmetric origin, still exist for that uniform model profile. Thus, for the order parameter, which is independent of the spatial coordinate up to the surface or interface, one can find in the tunneling limit only peak at zero energy in the local density of states, while all nonzero peaks taking place in the presence of surface pair breaking turn out to disappear in the model.

Bound states with nonzero energy result in the anomalies of current-voltage characteristics in the presence of externally applied voltage, described in Refs. 2 and 7 and entirely omitted in Ref. 1. Positions and characteristics of those anomalies turn out to be associated with positions and types of extremal points of momentum dependence (dispersion) of bound state energies. We note that even in the absence of any surface pair breaking there are some additional peaks and jumps of the conductance of the SIS junction, involving anisotropically paired superconductors. Positions of the specific features of the conductance are determined by the extremal points of the sum of order parameters on both sides of the junction (and for the difference as well, although not for sufficiently low temperatures), taken for incoming and transmitted quasiparticle momenta.[2] These specific features are omitted in Ref. 1 as well.

Midgap states are dispersionless bound states. Their contributions to junction characteristics can differ from the ones with nonzero energy. The effect of finite transmission of the barrier plane beyond the tunneling limit may result in a shift of the interface bound states on account of both the phase difference of the order parameters and the surface pair breaking. In particular, a shift of midgap states to nonzero energies, in general, takes place on account of a finite transmission. These ‘‘former midgap states’’ take place for the uniform model as well.

Neglecting the surface pair breaking is the common feature of many articles, which consider surface (interface) bound states in d-wave superconductors both in studying current-voltage characteristics[1,9–14] and the dc Josephson effect.[15–17] It is worth noting that the effect of surface pair breaking can be of importance not only for studying the current-voltage characteristics but in considering the Josephson critical current as well. Since the low-temperature anomaly of the Josephson critical current is associated with the effect of midgap states,[6] the influence of surface pair breaking on the characteristics of midgap states should be discussed in this context. The occurrence of the zero-energy peak in the tunneling density of states is unaffected by the self-consistency of the order parameter. However, neglecting the surface pair breaking can result in substantial overestimating the weight of the peak and, as a consequence, the Josephson critical current. Moreover, since surface pair breaking is sensitive to the crystal to surface orientation, disregarding its effect results in qualitative changes in dependences of the peak height and I_c upon the misorientation angles of superconductors from both sides of the junction. For example, the midgap state contribution to the Josephson critical current between two identically oriented d-wave superconductors, calculated within the simple model for d-wave order parameter, reveals strong deviation of self-consistent angular dependence from the non-self-consistent one. The most significant deviation takes place for the misorientation angle $\theta = 45°$, when the order parameter is completely suppressed near the boundary. For this particular orientation disregarding the surface pair breaking results in the overestimation of the midgap contribution to the Josephson critical current by more than three times (see also Ref. 18 and Fig. 2 in Ref. 19). This leads, in particular, to the failure of the simple orientation dependence $I_c(\text{midgap}) \propto \sin(2\theta_1)\sin(2\theta_2)$, obtained in Refs. 17 and 1 on the basis of a uniform model for the order parameter and some additional approximations. One can show, however, that signs of $I_c(\text{midgap})$ and $\sin(2\theta_1)\sin(2\theta_2)$ coincide for the particular pairing potential considered.

We should mention as well a substantial drawback of the model, associated with the particular form of the order parameter in Eq. (25) in Ref. 1 which was used there in the numerical calculations. This form does not correspond to a $d_{x^2-y^2}$-wave superconductor and could only arise from mixing in $d_{x^2-y^2}$- and d_{xy}-wave order parameters in the bulk of a superconductor. This form requires for the self-consistency pairing interactions between both near-neighbor and next-nearest-neighbor quasiparticles on a tetragonal lattice, which leads to a different quasiparticle spectrum as compared to a tight-binding form used in Ref. 1. This leads, in general, to distinctively different results. This effect was studied in detail by the authors of Refs. 4 and 5.

Even a correct consideration of the problem in question within such a simplified model like a model for a superconductor with a cylindrical Fermi surface, encounters a question on possible modifications of the results due to realistic, probably, complicated forms of the Fermi surfaces of the particular compounds considered. One can expect the actual forms of the Fermi surfaces to modify substantially both the pairing states and the particular conditions leading to the appearance of the surface quasiparticle bound states. Interestingly, if one assumes the presence of the surface bound states, then the problem of unconventional features of the current-voltage characteristics of tunnel junctions they bring about can be solved (even analytically) under quite general conditions. It turns out that the answer does not depend on the particular forms of the Fermi surfaces, but is governed mostly by their dimensionalities and the types of the extremal points of the dispersion dependences of the surface bound states.[2,7]

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